

An asymptotic preserving scheme for kinetic models for chemotaxis phenomena

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Abstract

In this paper, we propose a numerical scheme to solve the kinetic model for chemotaxis phenomena. Formally, this scheme is shown to be uniformly stable with respect to the small parameter, consistent with the fluid-diffusion limit (Keller-Segel model). Our approach is based on the micro-macro decomposition which leads to an equivalent formulation of the kinetic model that couples a kinetic equation with macroscopic ones. This method is validated with various test cases and compared to other standard methods.

keyword: Asymptotic preserving scheme; Kinetic theory; Micro-macro decomposition; Chemotaxis phenomena

MSC: 65M06, 35Q20, 82C22, 92B0

1 Introduction

Chemotaxis is a process by which cells change their state of movement reacting to the presence of a chemical substance, approaching chemically favorable environments and avoiding unfavorable ones. In the simple situation where we only consider cells and a chemical substance (the chemo-attractant), a model for the space and time evolution of the density $n = n(t, x)$ of cells and the chemical concentration $S = S(t, x)$ at time t and position x has been introduced by Patlak [41] and Keller-Segel [30] reads:

$$\begin{cases} \frac{\partial n}{\partial t} + \nabla_x \cdot (n \chi(S) \cdot \nabla_x S - D_n \cdot \nabla_x n) = 0, \\ \frac{\partial S}{\partial t} - D_S \Delta S = H(n, S), \end{cases} \quad (1)$$

where ∇_x denotes the gradient with respect to the spatial variable, and the positive constants D_S and D_n are the diffusivity of the chemo-attractant and of the cells, respectively, and χ is the chemotactic sensitivity.

In general the substance S does not only diffuse in the substrate, but it can also be produced by the bacteria themselves. The role of the function $H(n, S)$ is to describe the interaction between both quantities. One typical example is given by

$$H(n, S) = an - bS, \quad (2)$$

which describes the production of the chemo-attractant by the bacteria at a constant rate a as well as chemical decay with relaxation time $\frac{1}{b}$. Since the bacterial movement is directed toward the higher concentrations of S , the coupling is attractive. A deep insight into the phenomenological derivation of Keller and Segel types models is given in the survey [23].

The behavior of this system is now quite wellknown: in the one-dimensional case, the solution is always global in time. In several space dimensions, if initial data are small enough in some norms, the solution will be global in time and rapidly decaying in time; while on the opposite, it will explode in finite time at least for some large initial data. The simplicity, the analytical tractability, and the capacity to replicate some of the key behaviors of chemotactic populations are the main reasons of the success of this model of chemotaxis. In particular, the ability to display auto-aggregation, has led to its prominence as a mechanism for self-organization of biological systems. Moreover, there exists a lot of variations of system (1) to describe biological processes in which chemotaxis is involved. They differ in the functional forms of the three main mechanisms involved in the chemotactical movement. They are: the sensing of the chemoattractant, which has an effect on the oriented movement of the species, the production of the chemoattractant by a mobile species or an external source, and the degradation of the chemoattractant by a mobile species or an external effect. The surveys [24] and [5] provide a detailed review and critical analysis of the qualitative properties of the solutions to problems related to the application of Keller and Segel models to various biological contexts.

Another point of view was introduced by a mesoscopic description of these phenomena bridging from stochastic interacting particle systems to macroscopic equations. This middle ground consists in describing the movement of cells by a "run & tumble" process [35, 36]. The cells move along a straight line in the running phase and make reorientation as a reaction to the surrounding chemicals during the tumbling phase. This is the typical behavior that has been observed in experiments. The resulting nondimensionalized kinetic equation, with parabolic rescaling, reads

$$\begin{cases} \varepsilon \frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\varepsilon} \mathcal{T}(S, f), \\ \frac{\partial S}{\partial t} - D_S \Delta S = H(n, S), \\ f(0, x, v) = f_0(x, v), \end{cases} \quad (3)$$

where $f(t, x, v)$ denotes the density of cells, depending on time t , position $x \in \Omega \subset \mathbb{R}^d$ and velocity $v \in V \subset \mathbb{R}^d$. \mathcal{T} is an operator, which models the change of direction of cells and ε is a time scale which here refers to the turning frequency.

The function $S(t, x)$ is the chemical concentration, where n denotes the density of cells, and is given by

$$n(t, x) = \int_V f(t, x, v) dv. \quad (4)$$

Starting with the kinetic equation (3), one can (at least formally) derive the macroscopic limit (1) as $\varepsilon \rightarrow 0$. The details will be described in Section 3. Other asymptotic limits, such as the hyperbolic limits have been investigated in Refs [1, 2, 3, 6, 19, 22].

The general context of this paper is the development of numerical schemes for solving the kinetic equation that are uniformly stable along the transition from kinetic regime to the fluid regime. The main difficulty is due to the term $\frac{1}{\varepsilon}$ which becomes stiff when ε is close to zero (macroscopic regime). In this case, solving the kinetic equation by a standard explicit numerical scheme requires the use of a time step of the order of ε , which leads to very expensive numerical computations for small ε . To avoid this difficulty, it is necessary to use an implicit or semi-implicit time discretization for the collision part. In fact, such numerical schemes should also have a correct asymptotic behavior: for small parameter ε , the schemes should degenerate into a good approximation of the asymptotics (Keller-Segel model) of the kinetic equation. This property is often called "asymptotic preserving", and has been introduced in [26] for numerical schemes that are stable with respect to a small parameter ε and degenerate into a consistent numerical scheme for the limit model when $\varepsilon \rightarrow 0$.

Considering that this paper deals with asymptotic preserving scheme (AP), one also has to mention that there are different approaches to construct such schemes for kinetic models in various contexts. We mention for instance works based on domain decompositions, separating the macroscopic (fluid) domain from the microscopic (kinetic) one (see [14, 16]). There is another kind of (AP) schemes for kinetic equations, which are based on the use of time relaxed techniques where the Boltzmann collision operator is discretized by a spectral or a Monte-Carlo method (see [20, 38, 39, 40]). Other techniques have also been developed to design multiscale numerical methods which are based on splitting strategy [12, 27, 28, 31], penalization procedure [17, 18, 29, 43] or micro-macro decomposition which first was used by Liu and Yu for theoretical study of the fluid limit of the Boltzmann equation [34]. It was then used to develop an AP scheme for different asymptotics (diffusion, fluid, high-field, ...), see [7, 8, 9, 13, 15, 25, 32, 33].

In this work, we extend a method of micro-macro decomposition in order to construct asymptotic preserving schemes (AP) for kinetic equations describing chemotaxis phenomena. Our strategy consists in rewriting the kinetic equation as a coupled system of kinetic part and macroscopic one, by using the micro-macro decomposition of the distribution function. Indeed, this function is decomposed into its corresponding equilibrium distribution plus the deviation. By using a classical projection technique, we obtain an evolution equation for the macroscopic parameters of the equilibrium coupled to a kinetic equation for the non-equilibrium part. Although our approach is rather general to apply

to a very large class of collision operators, the numerical tests shown in our work were obtained with very simple model.

The outline of this paper is the following. In Sect. 2, we present the kinetic model and its properties. The micro-macro decomposition, the corresponding formulation of the kinetic equation, and the macroscopic limit are presented in Sect. 3. Our numerical scheme is presented in Sect. 4. Finally, our method is demonstrated with a numerical tests in Sect. 5.

2 The kinetic model

In this section we briefly describe the kinetic models we used. The turning kernel \mathcal{T} in the kinetic equation (3) needs to be specified. The turning kernel, \mathcal{T} measures the probability of velocity jump of cells from v' to v . To derive the Keller- Segel equation (1) as $\varepsilon \rightarrow 0$, one has to incorporate both $O(1)$ and $O(\varepsilon)$ scale into \mathcal{T} . In the following work, as in [1, 19, 21, 37] we assume herein that the turning operator is of the form

$$\mathcal{T}(S, f) = \mathcal{T}_0(f) + \varepsilon \mathcal{T}_1(S)(f), \quad (5)$$

where \mathcal{T}_0 represents the dominant part of the turning kernel modeling the tumble process in the absence of chemical substance, supposed independent of S and $\mathcal{T}_1(S)$ is the perturbation due to chemical cues. We first mention some assumptions on the turning operators \mathcal{T}_0 and $\mathcal{T}_1(S)$:

- The operators \mathcal{T}_0 and \mathcal{T}_1 preserve the local mass:

$$\int_V \mathcal{T}_0(f) dv = \int_V \mathcal{T}_1(S, f) dv = 0, \quad (6)$$

for any $S \geq 0$.

- There exists a bounded velocity distribution $M(v) > 0$, independent of x and t , such that:

1. The flow produce by the equilibrium distribution M vanishes, and M is normalized:

$$\int_V v M(v) dv = 0, \quad \int_V M(v) dv = 1. \quad (7)$$

2. The detailed balance

$$T_0(v', v)M(v) = T_0(v, v')M(v') \quad (8)$$

holds.

3. The kernel $T_0(v, v')$ is bounded, and there exists a constant $\sigma > 0$ such that

$$T_0(v, v') \geq \sigma M, \quad \forall (v, v') \in V \times V, \quad x \in \mathbb{R}^d, \quad t > 0. \quad (9)$$

The most commonly used assumption on the turning operators \mathcal{T}_i , $i = 0, 1$, is that they are both linear integral operators with respect to f and read:

$$\mathcal{T}_i(S, f) = \int_V (T_i(S, v, v')f(t, x, v') - T_i(S, v', v)f(t, x, v))dv'. \quad (10)$$

Here the turning kernel $T_1(S, v, v')$ describes the reorientation of cells, i.e. the random velocity changes from v to v' and may depend on the chemo-attractant concentration and its derivatives.

Technical calculations (see [1, 11]), namely by integration over v , interchanging v by v' , and using (8), yields the following equality:

$$\begin{aligned} \int_V \mathcal{T}_0(g) \frac{h(v)}{M(v)} dv &= \frac{1}{2} \int_V \int_V \Psi[M] \left(\frac{g(v')}{M(v')} - \frac{g(v)}{M(v)} \right) \\ &\quad \times \left(\frac{h(v)}{M(v)} - \frac{h(v')}{M(v')} \right) dv dv', \end{aligned} \quad (11)$$

where

$$\Psi[M] = \frac{1}{2} (T_0(v, v')M(v') + T_0(v', v)M(v)).$$

In particular Eq.(11) shows that the operators \mathcal{T}_0 , is a self-adjoint and the following equality:

$$- \int_V \mathcal{T}_0(h) \frac{h(v)}{M(v)} dv = \frac{1}{2} \int_V \int_V \Psi[M] \left(\frac{h(v)}{M(v)} - \frac{h(v')}{M(v')} \right)^2 dv dv' \geq 0 \quad (12)$$

holds true.

Moreover, for $\int_V h(v) dv = 0$, Eq.(12) and the estimate (9) yield the following inequality:

$$\begin{aligned} - \int_V \mathcal{T}_0(h) \frac{h(v)}{M(v)} dv &\geq \frac{\sigma}{2} \int_V \int_V M(v)M(v') \left(\frac{h(v)}{M(v)} - \frac{h(v')}{M(v')} \right)^2 dv dv' \\ &\geq \sigma \int_V \frac{h^2(v)}{M(v)} dv, \end{aligned} \quad (13)$$

which shows that \mathcal{T}_0 is a Fredholm operator in the space $L^2(V, \frac{dv}{M(v)})$. Therefore, the following result defines the properties of the operator \mathcal{T}_0 :

Lemma 1. *Suppose that Assumptions (7)-(9) hold. Then, the following properties of the operators \mathcal{T}_0 hold true:*

- i) *The operator \mathcal{T}_0 is self-adjoint in the space $L^2\left(V, \frac{dv}{M}\right)$.*
- ii) *For $f \in L^2$, the equation $\mathcal{T}_0(g) = f$, has a unique solution $g \in L^2\left(V, \frac{dv}{M}\right)$, which satisfies*

$$\int_V g(v) dv = 0 \quad \text{if and only if} \quad \int_V f(v) dv = 0.$$

- iii) The equation $\mathcal{T}_0(g) = v M(v)$, has a unique solution that we call $\theta(v)$.
- iv) The kernel of \mathcal{T}_0 is $N(\mathcal{T}_0) = \text{vect}(M(v))$.

3 The micro-macro decomposition of the kinetic model and macroscopic limit

3.1 The micro-macro decomposition

Let (f, S) be a solution of (3). We decompose f as follows

$$f = M(v)n + \varepsilon g,$$

where n is the density given by (4). Then $\langle g \rangle = 0$, where $\langle g \rangle = \int_V g dv$, and one has:

$$\begin{aligned} \frac{\partial(Mn)}{\partial t} + \varepsilon \frac{\partial g}{\partial t} + \frac{1}{\varepsilon} v M \cdot \nabla_x n + v \cdot \nabla_x g &= \frac{1}{\varepsilon} \mathcal{T}_0^1(g) \\ &+ \frac{1}{\varepsilon} \mathcal{T}_1(S)(M(v)n) + \mathcal{T}_1^1(S)(g). \end{aligned} \quad (14)$$

Now, we use a projection technique to separate the macroscopic and microscopic quantities $n(t, x)$ and $g(t, x, v)$. Moreover, let P_M , denotes the orthogonal projection onto $N(\mathcal{T}_0)$. Then

$$P_M(h) = \langle h \rangle M, \quad \text{for any } h \in L^2(V, \frac{dv}{M(v)}),$$

so that one has the following:

Lemma 2. *One has the following properties for the projection P_M :*

$$\begin{aligned} (I - P_M)(Mn) &= P_M(g) = 0, \\ (I - P_M)(v M \cdot \nabla_x n) &= v M \cdot \nabla_x n, \\ (I - P_M)(\mathcal{T}_1(S)(M(v)n)) &= \mathcal{T}_1(S)(M(v)n), \\ (I - P_M)(\mathcal{T}_1(S)(g)) &= \mathcal{T}_1(S)(g). \end{aligned}$$

Proof. The firsts equalities are trivials since $P_M(M) = M$, and $\langle g \rangle = 0$. As the flux produced by M is zero then $(I - P_M)(v M \cdot \nabla_x n) = v M \cdot \nabla_x n$. By using (6), one deduce that $P_M(\mathcal{T}_1(S)(h)) = 0$ for any $h \in L^2$, and then the third and the fourth equality are completed. \square

Taking the operator $I - P_M$ into the equation (14) and using Lemma 2, one deduce

$$\varepsilon \frac{\partial g}{\partial t} + \frac{1}{\varepsilon} v M \cdot \nabla_x n + (I - P_M)(v \cdot \nabla_x g) = \frac{1}{\varepsilon} \mathcal{T}_0(g) + \frac{1}{\varepsilon} \mathcal{T}_1(S)(M(v)n) + \mathcal{T}_1(S)(g). \quad (15)$$

Integrating (14) over v , yields

$$\frac{\partial n}{\partial t} + \langle v \cdot \nabla_x g \rangle = 0. \quad (16)$$

The micro-macro formulation finally reads:

$$\begin{cases} \varepsilon \frac{\partial g}{\partial t} + \frac{1}{\varepsilon} v M \cdot \nabla_x n + (I - P_M)(v \cdot \nabla_x g) = \frac{1}{\varepsilon} \mathcal{T}_0(g) + \frac{1}{\varepsilon} \mathcal{T}_1(S)(M(v)n) \\ \quad + \mathcal{T}_1(S)(g), \\ \frac{\partial n}{\partial t} + \langle v \cdot \nabla_x g \rangle = 0, \\ \frac{\partial S}{\partial t} - D_S \Delta S = H(n, S). \end{cases} \quad (17)$$

Equations (17) are the micro-macro formulation of the kinetic equation (3) that we want to use to design our AP scheme. The following proposition shows that this formulation is indeed equivalent to the kinetic equation (3).

Proposition 1.

1. Let (f, S) be a solution of (3) with initial data (f_0, S_0) . Then (n, g, S) , where $n = \langle f \rangle$ and $g = \frac{1}{\varepsilon}(f - M(v)n)$ is a solution to a coupled system (17) with the associated initial data:

$$\begin{cases} n(t=0) = n_0 = \langle f_0 \rangle, \\ g(t=0) = g_0 = \frac{1}{\varepsilon}(f_0 - M(v)n_0), \\ S(t=0) = S_0. \end{cases} \quad (18)$$

2. Conversely, if (n, g, S) satisfies system (17) with initial data (n_0, g_0, S_0) such that $\langle g_0 \rangle = 0$ then $f = M(v)n + \varepsilon g$ is a solution to kinetic model (3) with initial data $f_0 = M(v)n_0 + \varepsilon g_0$, and we have $n = \langle f \rangle$, and $\langle g \rangle = 0$.

Proof. The proof of i) is detailed above. For ii) consider (n, g, S) solution of (17). We set $f = M(v)n + \varepsilon g$ and we show that f is a solution of kinetic model (3). From (17), one has

$$\frac{\partial f}{\partial t} - M(v) \frac{\partial n}{\partial t} + \frac{1}{\varepsilon} v M \cdot \nabla_x n + v \cdot \nabla_x g - P_M(v \cdot \nabla_x g) = \frac{1}{\varepsilon^2} \mathcal{T}_0(f) + \frac{1}{\varepsilon} \mathcal{T}_1(S)(f),$$

and then

$$\frac{\partial f}{\partial t} - M(v) \frac{\partial n}{\partial t} + \frac{1}{\varepsilon} v \cdot \nabla_x f - M(v) \langle v \cdot \nabla_x g \rangle = \frac{1}{\varepsilon^2} \mathcal{T}_0(f) + \frac{1}{\varepsilon} \mathcal{T}_1(S)(f).$$

Therefore using (16), one obtains (3). The property $\langle g \rangle = 0$ is obtained by integrating (15) over v , using (6) and the property of the initial data. This completes the proof. \square

3.2 The macroscopic limit

In this subsection, the formal derivation of the macroscopic model is performed starting from the meso-macro model (3). The macroscopic model has been derived mathematically in [11]. Hereafter, we will see that the formal derivation is really straightforward starting from (17) (compared to the equivalent formulation of (3)), since the micro-macro model is well suited to deal with the asymptotic model in the diffusion limit. Indeed for small ε , the first equation of (17) by using (6) and (7) gives

$$g = \mathcal{T}_0^{-1}(vM \cdot \nabla_x n) - \mathcal{T}_0^{-1}(\mathcal{T}_1(S)(M(v)n)) + O(\varepsilon). \quad (19)$$

Inserting (19) into (16) yields the asymptotic model (coupled with the concentration equation for S):

$$\begin{cases} \frac{\partial n}{\partial t} + \langle v \cdot \nabla_x (\mathcal{T}_0^{-1}(v \cdot \nabla_x n)) \rangle - \langle v \cdot \nabla_x (\mathcal{T}_0^{-1}(\mathcal{T}_1(S)(M(v)n))) \rangle = O(\varepsilon), \\ \frac{\partial S}{\partial t} - D_S \Delta S = H(n, S). \end{cases} \quad (20)$$

Using iii) of Lemma 1, one has as \mathcal{T}_0 is self adjoint operator in $L^2(\frac{dv}{M(v)})$ the following:

$$\begin{aligned} \langle v \cdot \nabla_x (\mathcal{T}_0^{-1}(\mathcal{T}_1(S)(M(v)n))) \rangle &= \left\langle \mathcal{T}_0(\theta(v)) \cdot \frac{\nabla_x}{M(v)} (\mathcal{T}_0^{-1}(\mathcal{T}_1(S)(M(v)n))) \right\rangle \\ &= \operatorname{div}_x \left\langle \frac{\theta(v)}{M(v)} n \mathcal{T}_1(S)(M(v)) \right\rangle, \end{aligned}$$

and then the macroscopic model (20) becomes

$$\begin{cases} \frac{\partial n}{\partial t} + \operatorname{div}_x (n \alpha(S) - D_n \cdot \nabla_x n) = O(\varepsilon), \\ \frac{\partial S}{\partial t} - D_S \Delta S = H(n, S), \end{cases} \quad (21)$$

where D_n and $\alpha(S)$ are given by

$$D_n = - \int_V v \otimes \theta(v) dv, \quad \alpha(S) = - \int_V \frac{\theta(v)}{M(v)} \mathcal{T}_1(S)(M)(v) dv. \quad (22)$$

The approach we have developed is quite general. The Keller-Segel model is now given.

3.3 The Keller-Segel model

Let us first consider the following task for the probability kernels:

$$T_0(v, v') = \sigma M(v), \quad \sigma > 0.$$

Consequently, the leading turning operators \mathcal{T}_0 become relaxation operators:

$$\mathcal{T}_0(g) = -\sigma (g - \langle g \rangle M). \quad (23)$$

In particular, θ and the diffusion tensor D_n are given by:

$$\theta(v) = -\frac{1}{\sigma} M(v), \quad D_n = \frac{1}{\sigma} \int_V v \otimes v M(v) dv. \quad (24)$$

Moreover $\alpha(S)$ is given by:

$$\alpha(S) = \frac{1}{\sigma} \int_V v \mathcal{T}_1[S](M(v)) dv. \quad (25)$$

The relaxation kernels presented in together with the choice

$$\mathcal{T}_1[S] = K_S(v, v') \cdot \nabla_x S,$$

where $K_S(v, v')$ is a vector valued function, leads to the model

$$\mathcal{T}_1[S](M) = h(v, S) \cdot \nabla_x S,$$

where

$$h(v, S) = \int_V \left(K_S(v, v') M(v') - K_S(v', v) M(v) \right) dv'.$$

Finally, the function $\alpha(S)$ in (25) is given by

$$\alpha(S) = \chi(S) \cdot \nabla_x S,$$

where the chemotactic sensitivity $\chi(S)$ is given by the matrix

$$\chi(S) = \frac{1}{\sigma} \int_V v \otimes h(v, S) dv. \quad (26)$$

Therefore, the drift term $\text{div}_x(n \alpha(S))$ that appears in the macroscopic case stated by (20) becomes:

$$\text{div}_x(n \alpha(S)) = \text{div}_x(n \chi(S) \cdot \nabla_x S),$$

which gives a Keller-Segel type model (1):

$$\begin{cases} \frac{\partial n}{\partial t} + \text{div}_x(n \chi(S) \cdot \nabla_x S - D_n \cdot \nabla_x n) = O(\varepsilon), \\ \frac{\partial S}{\partial t} - D_S \Delta S = H(n, S). \end{cases} \quad (27)$$

4 Numerical methods

Here in this section, we consider Problem (3), subject to the following initial conditions:

$$f(0, x, v) = f_0(x, v) \quad \text{and} \quad S(0, x) = S_0(x). \quad (28)$$

It has been shown that problem (3) is equivalent to the following micro-macro formulation:

$$\begin{cases} \frac{\partial g}{\partial t} + \frac{1}{\varepsilon^2} v M \cdot \nabla_x n + \frac{1}{\varepsilon} (I - P_M)(v \cdot \nabla_x g) = \frac{1}{\varepsilon^2} \mathcal{T}_0(g) \\ \quad + \frac{1}{\varepsilon^2} \mathcal{T}_1(S)(M(v)n) + \frac{1}{\varepsilon} \mathcal{T}_1(S)(g), \\ \frac{\partial n}{\partial t} + \langle v \cdot \nabla_x g \rangle = 0, \\ \frac{\partial S}{\partial t} - D_S \Delta S = H(n, S), \end{cases} \quad (29)$$

subject to the following initial conditions:

$$n(t=0) = n_0 = \langle f_0 \rangle, \quad g(t=0) = g_0 = \frac{1}{\varepsilon} (f_0 - M(v)n_0), \quad S(0, x) = S_0(x). \quad (30)$$

The discretization of problem (29)-(30) is carried out with respect to each independent variable (time, velocity and space).

4.1 Time discretization

The treatment of the time variable of problem (29)-(30) can be done by using varieties of methods such as finite difference and variational methods. Finite-differencing the derivative in time is the widely used approach.

The time interval $[0, T]$ is divided into N times steps as follows:

$$t_0 = 0, \quad t_{k+1} = t_k + \Delta t, \quad 0 \leq k < N,$$

where $\Delta t = \frac{T}{N}$ is the time step. The approximation of $n(t, x)$ and $g(t, x, v)$ at the time step t_k are denoted respectively by $n^k \approx n(t_k, x)$ and $g^k \approx g(t_k, x, v)$. Using an implicate scheme for the stiff term $\frac{1}{\varepsilon^2} \mathcal{T}_0(g)$ and an explicite for the other terms in the first equation in (29), one obtains :

$$\begin{aligned} \frac{g^{k+1} - g^k}{\Delta t} &= -\frac{1}{\varepsilon^2} v M \cdot \nabla_x n^k - \frac{1}{\varepsilon} (I - P_M)(v \cdot \nabla_x g^k) \\ &+ \frac{1}{\varepsilon^2} \mathcal{T}_0(g^{k+1}) + \frac{1}{\varepsilon^2} \mathcal{T}_1(S^k)(M(v)n^k) \\ &+ \frac{1}{\varepsilon} \mathcal{T}_1(S^k)(g^k). \end{aligned} \quad (31)$$

Substituting g by g^{k+1} in the second equation of (29) yields

$$\frac{n^{k+1} - n^k}{\Delta t} + \langle v \cdot \nabla_x g^{k+1} \rangle = 0. \quad (32)$$

Replacing n in the third equation by n^{k+1} one has:

$$\frac{S^{k+1} - S^k}{\Delta t} - D_S \Delta S^{k+1} = H(n^{k+1}, S^{k+1}). \quad (33)$$

Proposition 2. *The time discretization (31)-(32) of the first and second equation of system (29) is consistent with the first equation of system (20) when $\varepsilon \rightarrow 0$.*

Proof. Formally, we have from (31):

$$\begin{aligned} \left(I - \frac{\Delta t}{\varepsilon^2} \mathcal{T}_0\right) g^{k+1} &= g^k + \frac{\Delta t}{\varepsilon^2} [\mathcal{T}_1(S^k)(M(v)n^k + \varepsilon g^k) - vM \cdot \nabla_x n^k \\ &\quad - \varepsilon(I - P_M)v \cdot \nabla_x g^k]. \end{aligned} \quad (34)$$

Since the operator $-\mathcal{T}_0$ is self adjoint and positive, $(I - \frac{\Delta t}{\varepsilon^2} \mathcal{T}_0)$ is self-adjoint and positive definite thus invertible for $\Delta t > 0$. Therefore one has

$$\begin{aligned} g^{k+1} &= \left(I - \frac{\Delta t}{\varepsilon^2} \mathcal{T}_0\right)^{-1} \left(g^k + \frac{\Delta t}{\varepsilon^2} [\mathcal{T}_1(S^k)(M(v)n^k + \varepsilon g^k) - vM \cdot \nabla_x n^k \right. \\ &\quad \left. - \varepsilon(I - P_M)v \cdot \nabla_x g^k]\right). \end{aligned} \quad (35)$$

Developing the right hand side of (35) with regard to ε when $\varepsilon \rightarrow 0$, yields:

$$g^{k+1} = \mathcal{T}_0^{-1} [vM \cdot \nabla_x n^k] - \mathcal{T}_0^{-1} [\mathcal{T}_1(S^k)(M(v)n^k)] + O(\varepsilon). \quad (36)$$

Substituting g^{k+1} in (32) leads to

$$\frac{n^{k+1} - n^k}{\Delta t} + \langle v \cdot \nabla_x \mathcal{T}_0^{-1} [vM \cdot \nabla_x n^k] \rangle - \langle v \cdot \nabla_x \mathcal{T}_0^{-1} [\mathcal{T}_1(S^k)(M(v)n^k)] \rangle = O(\varepsilon), \quad (37)$$

which is consistent with the first equation of system (20) when $\varepsilon \rightarrow 0$. \square

4.2 Spatial discretization and velocity discretization

In the following, we present the methods in the case of 1-dimensional spatial and velocity discretization. The phase-space interval is denoted by $[x_{min}, x_{max}] \times [v_{min}, v_{max}]$, where $-v_{min} = v_{max} > 0$.

4.2.1 Spatial discretization

For the spatial discretization, a difference method based on control volume approach and cell averaging is used. The numerical grid is defined by:

$$R_{\Delta x} = \{x_i, x_{i+\frac{1}{2}}, \quad 0 \leq i \leq N_x = \frac{x_{max} - x_{min}}{\Delta x}\}, \quad (38)$$

where $\Delta x > 0$ is the spatial mesh size, $x_0 = x_{min}$, $x_i = x_{i-1} + \Delta x$ ($1 \leq i \leq N_x$) and $x_{i+\frac{1}{2}} = (x_{i+1} + x_i)/2$ ($0 \leq i \leq N_x - 1$) are the cell center points. Proceeding as in [8], the microscopic equation (31) is discretized at points $x_{i+\frac{1}{2}}$ while the macroscopic equation (32) and the diffusion equation (33) are discretized at points x_i . The approximation of $n(t, x)$, $g(t, x, v)$ and $S(t, x)$ at the considered

spatial points and at the time step t_k are denoted by $n_i^k \approx n(t_k, x_i)$, $g_{i+\frac{1}{2}}^k(v) \approx g(t_k, x_{i+\frac{1}{2}}, v)$ and $S_i^k \approx S(t_k, x_i)$ respectively.

Setting $v^+ = \max(0, v)$, $v^- = \min(0, v)$, the following spatially discrete forms are obtained:

$$\begin{aligned} & \frac{g_{i+\frac{1}{2}}^{k+1} - g_{i+\frac{1}{2}}^k}{\Delta t} + \frac{1}{\varepsilon}(I - P_M) \left(v^+ \frac{g_{i+\frac{1}{2}}^k - g_{i-\frac{1}{2}}^k}{\Delta x} + v^- \frac{g_{i+\frac{3}{2}}^k - g_{i+\frac{1}{2}}^k}{\Delta x} \right) \\ &= \frac{1}{\varepsilon^2} \left(\mathcal{T}_0(g_{i+\frac{1}{2}}^{k+1}) + \mathcal{T}_1(S_{i+\frac{1}{2}}^k)(M(v)n_{i+\frac{1}{2}}^k) - vM \cdot \frac{n_{i+1}^k - n_i^k}{\Delta x} \right) \\ &+ \frac{1}{\varepsilon} \mathcal{T}_1(S_{i+\frac{1}{2}}^k)(g_{i+\frac{1}{2}}^k), \end{aligned} \quad (39)$$

$$\frac{n_i^{k+1} - n_i^k}{\Delta t} + \left\langle v \frac{g_{i+\frac{1}{2}}^{k+1} - g_{i-\frac{1}{2}}^{k+1}}{\Delta x} \right\rangle = 0, \quad (40)$$

and

$$\frac{S_i^{k+1} - S_i^k}{\Delta t} - D_{S_i^k} \frac{S_{i-1}^{k+1} - 2S_i^{k+1} + S_{i+1}^{k+1}}{(\Delta x)^2} = H(n_i^{k+1}, S_i^{k+1}). \quad (41)$$

Proposition 3. *From the discretization (39)-(41) of (3), yields the following numerical scheme when $\varepsilon \rightarrow 0$:*

$$\begin{aligned} & \frac{n_i^{k+1} - n_i^k}{\Delta t} + \frac{1}{\Delta x} \left\langle v \left[\mathcal{T}_0^{-1} \left(vM \cdot \frac{n_{i+1}^k - n_i^k}{\Delta x} \right) \right. \right. \\ & \quad \left. \left. - \mathcal{T}_0^{-1} \left(vM \cdot \frac{n_i^k - n_{i-1}^k}{\Delta x} \right) \right] \right\rangle \\ & \quad - \frac{1}{\Delta x} \left\langle v \left[\mathcal{T}_0^{-1} \left(\mathcal{T}_1(S_{i+\frac{1}{2}}^k)(M(v)n_{i+\frac{1}{2}}^k) \right) \right. \right. \\ & \quad \left. \left. - \mathcal{T}_0^{-1} \left(\mathcal{T}_1(S_{i-1/2}^k)(M(v)n_{i-1/2}^k) \right) \right] \right\rangle = 0 \end{aligned} \quad (42)$$

which is consistent with the first equation of system (20). Moreover, the approximation of the diffusion term is second order accurate in space.

Proof. The quantity $g_{i+\frac{1}{2}}^k$ is derived from (39) as:

$$\begin{aligned} g_{i+\frac{1}{2}}^{k+1} &= \left(I - \frac{\Delta t}{\varepsilon^2} \mathcal{T}_0 \right)^{-1} \left[g_{i+\frac{1}{2}}^k \right. \\ & \quad - \frac{\Delta t}{\varepsilon} (I - P_M) \left(v^+ \frac{g_{i+\frac{1}{2}}^k - g_{i-\frac{1}{2}}^k}{\Delta x} + v^- \frac{g_{i+\frac{3}{2}}^k - g_{i+\frac{1}{2}}^k}{\Delta x} \right) \\ & \quad + \frac{\Delta t}{\varepsilon^2} \left(\varepsilon \mathcal{T}_1(S_{i+\frac{1}{2}}^k)(g_{i+\frac{1}{2}}^k) + \mathcal{T}_1(S_{i+\frac{1}{2}}^k)(M(v)n_{i+\frac{1}{2}}^k) \right. \\ & \quad \left. \left. - vM \cdot \frac{n_{i+1}^k - n_i^k}{\Delta x} \right) \right]. \end{aligned}$$

It follows that:

$$g_{i+\frac{1}{2}}^{k+1} = \mathcal{T}_0^{-1} \left[vM \cdot \frac{n_{i+1}^k - n_i^k}{\Delta x} - \mathcal{T}_1(S_{i+\frac{1}{2}}^k)(M(v)n_{i+\frac{1}{2}}^k) \right] + O(\varepsilon) \quad (43)$$

as $\varepsilon \rightarrow 0$. Replacing $g_{i+\frac{1}{2}}^{k+1}$ in (40) by its expression of (43) and passing to the limit yields the relation (42). Proceeding as in the continuous case, the spatially discrete form (42) is consistent with the first equation of system (20). \square

4.2.2 Velocity discretization

We consider a uniform velocity grid defined as:

$$V_{\Delta v} = \{v_j = v_{min} + j\Delta v, 0 \leq j \leq N_v\}, \quad (44)$$

where $\Delta v = \frac{v_{max} - v_{min}}{N_v}$ is the velocity step and $N_v \in \mathbb{N}^*$ is an odd number. The approximation of $g(t, x, v)$ at the spatial points $x_{i+\frac{1}{2}}$ and velocity v_j at time step t_k is denoted by $g_{i+\frac{1}{2},j}^k \approx g(t_k, x_{i+\frac{1}{2}}, v_j)$. The phase-space discrete formulation of system (17) writes:

$$\begin{aligned} & \frac{g_{i+\frac{1}{2},j}^{k+1} - g_{i+\frac{1}{2},j}^k}{\Delta t} + \frac{1}{\varepsilon}(I - P_{M_j}) \left(v_j^+ \frac{g_{i+\frac{1}{2},j}^k - g_{i-\frac{1}{2},j}^k}{\Delta x} + v_j^- \frac{g_{i+\frac{3}{2},j}^k - g_{i+\frac{1}{2},j}^k}{\Delta x} \right) \\ &= \frac{1}{\varepsilon^2} \left(\mathcal{T}_{0,j}(g_{i+\frac{1}{2}}^{k+1}) + \mathcal{T}_{1,j}(S_{i+\frac{1}{2}}^k)(M(v_j)n_{i+\frac{1}{2}}^k) - v_j M(v_j) \cdot \frac{n_{i+1}^k - n_i^k}{\Delta x} \right) \\ &+ \frac{1}{\varepsilon} \mathcal{T}_{1,j}(S_{i+\frac{1}{2}}^k)(g_{i+\frac{1}{2}}^k), \end{aligned} \quad (45)$$

$$\frac{n_i^{k+1} - n_i^k}{\Delta t} + \left\langle v_j \frac{g_{i+\frac{1}{2},j}^{k+1} - g_{i-\frac{1}{2},j}^{k+1}}{\Delta x} \right\rangle = 0, \quad (46)$$

and

$$\frac{S_i^{k+1} - S_i^k}{\Delta t} - D_{S_i^k} \frac{S_{i-1}^{k+1} - 2S_i^{k+1} + S_{i+1}^{k+1}}{\Delta x^2} = G(n_i^{k+1}, S_i^{k+1}), \quad (47)$$

$0 \leq k < N$, $0 \leq i < N_x$, and $0 \leq j \leq N_v$.

In the discrete case, the bracket $\langle \cdot \rangle$, the projection $I - P_{M_j}$ and the integral operators $\mathcal{T}_{0,j}$ and $\mathcal{T}_{1,j}(S_{i+\frac{1}{2}}^k)$ are defined by:

$$\langle G_j \rangle = \Delta v \sum_{j=0}^{N_v-1} \bar{G}_j, \quad (48)$$

$$(I - P_{M_j})(G_j) = G_j - M_j \Delta v \sum_{k=0}^{N_v-1} \bar{G}_k, \quad (49)$$

$$\mathcal{T}_{0,j}(G) = \Delta v \left(\sum_{l=0}^{N_v-1} T_0(v_j, \bar{v}_l) \bar{G}_l - G_j \sum_{l=0}^{N_v-1} T_0(\bar{v}_l, v_j) \right), \quad (50)$$

and

$$\mathcal{T}_{1,j}(S_{i+\frac{1}{2}}^k)(G) = \Delta v \left(\sum_{l=0}^{N_v-1} T_1(S_{i+\frac{1}{2}}^k, v_j, \bar{v}_l) \bar{G}_l - G_j \sum_{l=0}^{N_v-1} T_1(S_{i+\frac{1}{2}}^k, \bar{v}_l, v_j) \right), \quad (51)$$

where $\bar{u}_j = (u_j + u_{j+1})/2$.

4.2.3 Boundary condition

For the numerical solution of the kinetic equation (3), the following inflow boundary conditions are usually prescribe for the distribution function f :

$$f(t, x_{min}, v) = f_l(v), \quad v > 0 \quad \text{and} \quad f(t, x_{max}, v) = f_r(v), \quad v < 0, \quad (52)$$

which can be rewritten in the micro-macro formulation:

$$\begin{aligned} n(t, x_0)M_j + \frac{\varepsilon}{2} \left(g(t, x_{\frac{1}{2}}, v_j) + g(t, x_{-\frac{1}{2}}, v_j) \right) &= f_l(v_j), & v_j > 0, \\ n(t, x_{N_x})M_j + \frac{\varepsilon}{2} \left(g(t, x_{N_x+\frac{1}{2}}, v_j) + g(t, x_{N_x-\frac{1}{2}}, v_j) \right) &= f_r(v_j), & v_j < 0. \end{aligned} \quad (53)$$

The following artificial Neumann boundary conditions are imposed for the other velocities [15]:

$$\begin{aligned} g(t, x_{-\frac{1}{2}}, v_j) &= g(t, x_{\frac{1}{2}}, v_j), & v_j < 0, \\ g(t, x_{N_x+\frac{1}{2}}, v_j) &= g(t, x_{N_x-\frac{1}{2}}, v_j), & v_j > 0. \end{aligned} \quad (54)$$

Therefore, the "ghost" points can be computed as follows:

$$g_{-\frac{1}{2},j}^{k+1} = \begin{cases} \frac{2}{\varepsilon} (f_l(v_j) - n_0^{k+1} M_j) - g_{\frac{1}{2},j}^{k+1}, & v_j > 0, \\ g_{\frac{1}{2},j}^{k+1}, & v_j < 0, \end{cases} \quad (55)$$

$$g_{N_x+\frac{1}{2},j}^{k+1} = \begin{cases} \frac{2}{\varepsilon} (f_r(v_j) - n_{N_x}^{k+1} M_j) - g_{N_x-\frac{1}{2},j}^{k+1}, & v_j < 0, \\ g_{N_x-\frac{1}{2},j}^{k+1}, & v_j > 0. \end{cases} \quad (56)$$

It then follows from (46) that:

$$\left(1 + \frac{2\Delta t}{\varepsilon \Delta x} \langle v_j^+ M_j \rangle \right) n_0^{k+1} = n_0^k - \frac{\Delta t}{\Delta x} \left\langle (v_j + v_j^+ - v_j^-) g_{\frac{1}{2},j}^{k+1} - \frac{2v_j^+}{\varepsilon} f_l(v_j) \right\rangle, \quad (57)$$

and

$$\begin{aligned} \left(1 - \frac{2\Delta t}{\varepsilon \Delta x} \langle v_j^- M_j \rangle \right) n_{N_x}^{k+1} &= n_{N_x}^k - \frac{\Delta t}{\Delta x} \left\langle \frac{2v_j^-}{\varepsilon} f_r(v_j) \right. \\ &\quad \left. - (v_j - v_j^+ + v_j^-) g_{N_x-\frac{1}{2},j}^{k+1} \right\rangle. \end{aligned} \quad (58)$$

Additionally, the homogeneous Neumann boundary conditions are prescribed for the concentration S :

$$S_{-1}^{k+1} = S_1^{k+1} \quad \text{and} \quad S_{N_x+1}^{k+1} = S_{N_x-1}^{k+1}. \quad (59)$$

4.2.4 Implementation of the method

To implement our method, we consider H given by (2). At the time step t_k , let us define the following vectors:

$$\bar{M} = \begin{pmatrix} M(v_0) \\ M(v_1) \\ \vdots \\ M(v_{N_v}) \end{pmatrix}, \quad G^k = \begin{pmatrix} G_{\frac{1}{2}}^k \\ G_{\frac{3}{2}}^k \\ \vdots \\ G_{N_x-\frac{1}{2}}^k \end{pmatrix},$$

with

$$G_{i+\frac{1}{2}}^k = \left(g_{i+\frac{1}{2},0}^k, g_{i+\frac{1}{2},1}^k, \dots, g_{i+\frac{1}{2},N_v}^k \right)^T,$$

$$N_{in}^k = \begin{pmatrix} n_1^k \\ n_2^k \\ \vdots \\ n_{N_x-1}^k \end{pmatrix}, \quad S^k = \begin{pmatrix} S_0^k \\ S_1^k \\ \vdots \\ S_{N_x}^k \end{pmatrix} \quad \text{and} \quad F^k = \begin{pmatrix} F_0^k \\ F_1^k \\ \vdots \\ F_{N_x}^k \end{pmatrix},$$

with $F_i^k = a(\Delta t)n_i^{k+1}$.

Setting

$$w_{jl}^0 = \frac{\Delta t \Delta v}{\varepsilon^2} T_0(v_j, \bar{v}_l), \quad \sigma_j^0 = 1 + \frac{\Delta t \Delta v}{\varepsilon^2} \sum_{l=0}^{N_v-1} T_0(\bar{v}_l, v_j),$$

$$\alpha_{i,j}^{1k} = \sum_{l=0}^{N_v-1} T_1(S_{i+\frac{1}{2}}^k, \bar{v}_l, v_j), \quad \beta_{i,j,l}^{1k} = T_1(S_{i+\frac{1}{2}}^k, v_j, \bar{v}_l),$$

$$w_{i,j,l}^{1k} = \frac{\Delta t \Delta v}{\varepsilon} \beta_{i,j,l}^{1k}, \quad \sigma_{i,j}^{1k} = \frac{\Delta t \Delta v}{\varepsilon} \alpha_{i,j}^{1k},$$

$$w_{i,j,l}^{2k} = \frac{\Delta t \Delta v}{\varepsilon^2} \beta_{i,j,l}^{1k} n_{i+\frac{1}{2}}^k, \quad \sigma_{i,j}^{2k} = \frac{\Delta t \Delta v}{\varepsilon^2} \alpha_{i,j}^{1k} n_{i+\frac{1}{2}}^k + \left(\frac{(\Delta t) v_l}{\varepsilon^2} \right) \frac{n_{i+1}^k - n_i^k}{\Delta x},$$

then Eq. (45) can be recast as:

$$(A^0 - B^0)G_{i+\frac{1}{2}}^{k+1} = (B_i^{1k} - P^+ + P^- + I)G_{i+\frac{1}{2}}^k + B_i^{2k} \bar{M} + P^+ G_{i-\frac{1}{2}}^k - P^- G_{i+\frac{3}{2}}^k \quad (60)$$

for $0 \leq i \leq N_x - 1$, where

$$A_{j,l}^0 = \delta_{j,l} \sigma_{j-1}^0, \quad (1 \leq j, l \leq N_v + 1),$$

$$B_{j,1}^0 = \frac{w_{j-1,0}^0}{2}, \quad (1 \leq j \leq N_v + 1),$$

$$B_{j,l}^0 = w_{j-1,l-1}^0, \quad (1 \leq j \leq N_v + 1, 2 \leq l \leq N_v),$$

$$B_{j,N_v+1}^0 = \frac{w_{j-1,N_v}^0}{2}, \quad (1 \leq j \leq N_v + 1),$$

$$\begin{aligned}
B_{i,j,1}^{1k} &= \frac{w_{i,j-1,0}^{1k} - \delta_{j,1}\sigma_{i,j-1}^{1k}}{2}, \quad (1 \leq j \leq N_v + 1), \\
B_{i,j,l}^{1k} &= \frac{w_{i,j-1,l-1}^{1k} - \delta_{j,l}\sigma_{i,j-1}^{1k}}{2}, \quad (1 \leq j \leq N_v + 1, 2 \leq l \leq N_v), \\
B_{i,j,N_v+1}^{1k} &= \frac{w_{i,j-1,N_v}^{1k} - \delta_{j,N_v+1}\sigma_{i,j-1}^{1k}}{2}, \quad (1 \leq j \leq N_v + 1),
\end{aligned}$$

$$\begin{aligned}
B_{i,j,1}^{2k} &= \frac{w_{i,j-1,0}^{2k} - \delta_{j,1}\sigma_{i,0}^{2k}}{2}, \quad (1 \leq j \leq N_v + 1), \\
B_{i,j,l}^{2k} &= \frac{w_{i,j-1,l-1}^{2k} - \delta_{j,l}\sigma_{i,j-1}^{2k}}{2}, \quad (1 \leq j \leq N_v + 1, 2 \leq l \leq N_v), \\
B_{i,j,N_v+1}^{2k} &= \frac{w_{i,j-1,N_v}^{2k} - \delta_{j,N_v+1}\sigma_{i,N_v}^{2k}}{2}, \quad (1 \leq j \leq N_v + 1),
\end{aligned}$$

$$\begin{aligned}
P_{j,1}^{\pm} &= \frac{\frac{\Delta t}{\varepsilon \Delta x}(\delta_{j,1} - M_{j-1}(\Delta v)v_0^{\pm})}{2}, \quad (1 \leq j \leq N_v + 1), \\
P_{j,l}^{\pm} &= \frac{\frac{\Delta t}{\varepsilon \Delta x}(\delta_{j,l} - M_{j-1}(\Delta v)v_{l-1}^{\pm})}{2}, \quad (1 \leq j \leq N_v + 1, 2 \leq l \leq N_v), \\
P_{j,N_v+1}^{\pm} &= \frac{\frac{\Delta t}{\varepsilon \Delta x}(\delta_{j,N_v+1} - M_{j-1}(\Delta v)v_{N_v}^{\pm})}{2}, \quad (1 \leq j \leq N_v + 1).
\end{aligned}$$

Similarly, the vectors N_{in}^{k+1} and S^{k+1} are respectively computed from (46) and (47) as follows:

$$N_{in,i}^{k+1} = N_{in,i}^k - B(G_{i+\frac{1}{2}}^k - G_{i-\frac{1}{2}}^k), \quad i = 1, 2, \dots, N_x - 1, \quad (61)$$

and

$$A_k S^{k+1} = S^k + F^k, \quad (62)$$

where

$$A_k = \begin{pmatrix} a_{k0} & b_{k0} & & & \\ b_{k1} & a_{k1} & b_{k1} & & \\ & \ddots & \ddots & \ddots & \\ & & b_{kN_x-1} & a_{kN_x-1} & b_{kN_x-1} \\ & & & b_{kN_x} & a_{kN_x} \end{pmatrix},$$

with

$$\begin{cases} b_{k0} = -2c_0, \\ b_{ki} = -c_i, \quad i = 1, 2, \dots, N_x - 1, \\ b_{N_x} = -2c_{N_x}, \\ a_{ki} = (1 + 2c_i + b(\Delta t)), \quad i = 0, 1, \dots, N_x, \\ c_i = \frac{(\Delta t)D_{S^k}}{(\Delta x)^2}, \quad i = 0, 1, \dots, N_x, \end{cases}$$

and

$$B = \frac{\Delta t \Delta v}{\Delta x} \left(\frac{v_0}{2}, v_1, \dots, v_{N_v-1}, \frac{v_{N_v}}{2} \right).$$

The following algorithm is finally obtained for the numerical solution of the Micro-Macro system (17): Given G^0 , $G_{-\frac{1}{2}}^0$, $G_{N_x+\frac{1}{2}}^0$, S^0 , N_{in}^0 , n_0^0 , $n_{N_x}^0$.

For $k = 1, 2, \dots, N$

1. Solve $G_{i+\frac{1}{2}}^{k+1}$, ($i = 0, 1, \dots, N_x - 1$) from (60);
2. Compute N_{in}^{k+1} using (61);
3. Compute n_0^{k+1} and $n_{N_x}^{k+1}$ using (57) and (58);
4. Compute $G_{-\frac{1}{2}}^{k+1}$ and $G_{N_x+\frac{1}{2}}^{k+1}$ using (55);
5. Solve S^{k+1} from (62).

4.3 A time implicit discretization

The previous discretization is explicit of the macro part n . It then imposes the diffusion restriction on the time step $\Delta t = O((\Delta x)^2)$. To overcome this restriction, a time implicit discretization can be applied for the macro part such that at the limit, the diffusion term is treated implicitly. Following the idea in [15], a time implicit scheme can be derived the macro part of the micro-macro system. It consists to substitute $g_{i\pm\frac{1}{2}}^{k+1}$ in (40) by $\tilde{g}_{i\pm\frac{1}{2}}^{k+1}$ defined as follows:

$$\begin{aligned} \tilde{g}_{i+\frac{1}{2}}^{k+1} = & -\frac{\Delta t}{\varepsilon^2} \mathcal{H}_{0\varepsilon}^{-1} \left(vM \cdot \partial_x n_{i+\frac{1}{2}}^{k+1} \right) + \mathcal{H}_{0\varepsilon}^{-1} \left[g_{i+\frac{1}{2}}^k \right. \\ & - \frac{\Delta t}{\varepsilon} (I - P_M) \left(v^+ \frac{g_{i+\frac{1}{2}}^k - g_{i-\frac{1}{2}}^k}{\Delta x} + v^- \frac{g_{i+\frac{3}{2}}^k - g_{i+\frac{1}{2}}^k}{\Delta x} \right) \\ & \left. + \frac{\Delta t}{\varepsilon^2} \left(\varepsilon \mathcal{T}_1(S_{i+\frac{1}{2}}^k)(g_{i+\frac{1}{2}}^k) + \mathcal{T}_1(S_{i+\frac{1}{2}}^k)(M(v)n_{i+\frac{1}{2}}^k) \right) \right], \end{aligned} \quad (63)$$

where

$$\mathcal{H}_{0\varepsilon} = \left(I - \frac{\Delta t}{\varepsilon^2} \mathcal{T}_0 \right) \quad \text{and} \quad \partial_x n_{i+\frac{1}{2}}^{k+1} = \frac{n_{i+1}^{k+1} - n_i^{k+1}}{\Delta x}.$$

The following implicit time discretization of the macro part is obtained:

$$\begin{aligned} \frac{n_i^{k+1} - n_i^k}{\Delta t} - \left\langle \frac{\Delta t}{\varepsilon^2} v \mathcal{H}_{0\varepsilon}^{-1} \left(vM \frac{\partial_x n_{i+\frac{1}{2}}^{k+1} - \partial_x n_{i-\frac{1}{2}}^{k+1}}{\Delta x} \right) \right\rangle \\ + \left\langle v \frac{\hat{g}_{i+\frac{1}{2}}^{k+1} - \hat{g}_{i-\frac{1}{2}}^{k+1}}{\Delta x} \right\rangle = 0, \end{aligned} \quad (64)$$

where

$$\hat{g}_{i+\frac{1}{2}}^{k+1} = g_{i+\frac{1}{2}}^{k+1} + \frac{\Delta t}{\varepsilon^2} \mathcal{H}_{0\varepsilon}^{-1} \left(vM \cdot \partial_x n_{i+\frac{1}{2}}^k \right).$$

It can be seen that for small ε ,

$$\frac{\Delta t}{\varepsilon^2} \mathcal{H}_{0\varepsilon}^{-1} \left(vM \cdot \partial_x n_{i+\frac{1}{2}}^{k+1} \right) = -\mathcal{T}_0^{-1} \left(vM \cdot \partial_x n_{i+\frac{1}{2}}^{k+1} \right) + O(\varepsilon)$$

and

$$\hat{g}_{i+\frac{1}{2}}^{k+1} = \mathcal{T}_0^{-1} \left(\mathcal{T}_1(S^k)(M(v)n_{i+\frac{1}{2}}^k) \right).$$

Trough substitution and using the properties of \mathcal{T}_0 , we obtain the following discret form of the macro part as $\varepsilon \rightarrow 0$

$$\begin{aligned} \frac{n_i^{k+1} - n_i^k}{\Delta t} - D_n \frac{n_{i+1}^{k+1} - 2n_i^{k+1} + n_{i-1}^{k+1}}{(\Delta x)^2} \\ + \frac{\alpha(S_{i+\frac{1}{2}})n_{i+\frac{1}{2}}^k - \alpha(S_{i-\frac{1}{2}})n_{i-\frac{1}{2}}^k}{\Delta x} = 0, \end{aligned} \quad (65)$$

which is consistent with a discret form discretization of the macroscopic limit, using implicit discretization of the diffusion term. We remark that there is an additional computation of $\mathcal{H}_{0\varepsilon}^{-1}$ for the calculation of n^{k+1} . In the particular case where $\mathcal{T}_0(f) = -\sigma(f - \langle f \rangle M(v))$, we have from the micro-macro decomposition $\mathcal{T}_0(g_{i+\frac{1}{2}}^{k+1}) = -\sigma g_{i+\frac{1}{2}}^{k+1}$. Therefore

$$\begin{aligned} \frac{n_i^{k+1} - n_i^k}{\Delta t} - \frac{\Delta t}{\varepsilon^2 + \sigma \Delta t} \left\langle \left(v^2 M \frac{\partial_x n_{i+\frac{1}{2}}^{k+1} - \partial_x n_{i-\frac{1}{2}}^{k+1}}{\Delta x} \right) \right\rangle \\ + \left\langle v \frac{\hat{g}_{i+\frac{1}{2}}^{k+1} - \hat{g}_{i-\frac{1}{2}}^{k+1}}{\Delta x} \right\rangle = 0, \end{aligned} \quad (66)$$

and n^{k+1} is obtained by solving the linear system

$$(An^{k+1})_i = n_i^k - \Delta t \left\langle v \frac{\hat{g}_{i+\frac{1}{2}}^{k+1} - \hat{g}_{i-\frac{1}{2}}^{k+1}}{\Delta x} \right\rangle, \quad (67)$$

where A is the tridiagonal matrix $A = \text{Tridiag}(-\alpha, 2 + \alpha, -\alpha)$ with

$$\alpha = \langle v^2 M \rangle \frac{(\Delta x)^2}{(\Delta t)^2 (\varepsilon^2 + \Delta t)} \quad \text{and} \quad \hat{g}_{i+\frac{1}{2}}^{k+1} = g_{i+\frac{1}{2}}^{k+1} + \frac{\Delta t}{\varepsilon^2 + \sigma \Delta t} \left(vM \partial_x n_{i+\frac{1}{2}}^k \right).$$

The boundary conditions are incorporated using (57) and (58).

5 Numerical results

We present here some numerical experiments to validate our approach. In our tests, the space domain is the interval $X = [-1; 1]$, the velocity domain is $V = [-1; 1]$. For all the numerical tests carried out below, the velocity space is

divided into $N_v = 64$, which can provide good enough accuracy for numerical simulations [10]. The equilibrium distribution $M(v)$ and the kernels $T_0(v, v')$ and $T_1(S, v, v')$ are set to:

$$M(v) = \frac{1}{2}, \quad T_0(v, v') = M(v), \quad T_1(S, v, v') = (v \cdot \nabla S)_+.$$

It is clear that T_0 and T_1 satisfy assumptions (6)-(9). The boundary conditions are given by $f(t, -1, v) = 0, \forall v < 0; f(t, 1, v) = 0, \forall v > 0$. For the chemoattractant equation, we consider $H(n, S) = -S + n$ and the initial condition $S(0, x) = 0$. The initial condition for the cell density is a gaussian-like peak given as:

$$n(0, x) = C_M \exp(-80x^2),$$

where C_M is a constant determined such that the total mass is M . The initial cell distribution function is given as:

$$f(0, x, v) = \left(n(0, x) + \frac{v \exp(-v^2)}{C_M} \right) M(v).$$

We compare our scheme with:

- an Explicit-Euler scheme applied to the kinetic equation in the kinetic regime and to the diffusion equation in the Keller-Segel limit.
- an asymptotic preserving scheme obtained from a time splitting method applied to the Odd-Even decomposition of the kinetic equation in both kinetic and macroscopic regime.

• Explicit Euler scheme for the kinetic equation

The simplest time explicit scheme for the kinetic equation reads:

$$f_i^{k+1} = f_i^k - \frac{\Delta t}{\varepsilon \Delta x} (v^+(f_i^k - f_{i-1}^k) + v^-(f_{i+1}^k - f_i^k)) + \frac{\Delta t}{\varepsilon^2} \mathcal{T}(S^k, f_i^k). \quad (68)$$

Because of the stiff term $\varepsilon^{-2} \mathcal{T}(S^k, f_i^k)$, this scheme is not asymptotic preserving.

• Explicit Euler scheme for the Keller-Segel system

Under the above setting, the Keller-Segel system (27) reads:

$$\begin{cases} \frac{\partial n}{\partial t} = \partial_x (D \partial_x n - \chi n \partial_x S), \\ \frac{\partial S}{\partial t} = D_S \Delta S - S + n, \end{cases}$$

associated with homogenous Dirichlet boundary conditions for n (obtained from (53) when $\varepsilon \rightarrow 0$) and Neumann boundary conditions for S , where the coefficients D and χ are obtained from (24) and (26) respectively as $D_n = \frac{1}{3}$ and $\chi = \frac{1}{3}$.

The numerical solution to the first equation of the Keller-Seigel system can be computed by using the following standard explicit finite difference method [42]:

$$\frac{n_i^{k+1} - n_i^k}{\Delta t} = D \frac{n_{i+1}^k - 2n_i^k + n_{i-1}^k}{(\Delta x)^2} - \chi \frac{(\partial_x^{(c)} S_{i+1}^k) n_{i+1}^k - (\partial_x^{(c)} S_{i-1}^k) n_{i-1}^k}{\Delta x}, \quad (69)$$

where

$$\partial_x^{(c)} S_i^k = \frac{S_{i+1}^k - S_{i-1}^k}{2\Delta x}, \quad (1 \leq i \leq Nx - 1), \quad \partial_x^{(c)} S_0^k = \partial_x^{(c)} S_{Nx}^k = 0.$$

The diffusion term can also be treated implicitly in (69).

• **The Odd-Even parity decomposition asymptotic preserving scheme**

The Odd-Even decomposition asymptotic preserving scheme is based on the following parity equivalent form of the initial kinetic equation [10, 27]:

$$\begin{cases} \frac{\partial r}{\partial t} + v \partial_x j = \frac{1}{2\varepsilon^2} [(1 + \varepsilon |v \partial_x S|) n - (2 + \varepsilon |\partial_x S|) r], \\ \frac{\partial j}{\partial t} + \frac{1}{\varepsilon^2} v \partial_x r = \frac{1}{2\varepsilon^2} [(v \partial_x S) n - (2 + \varepsilon |\partial_x S|) j], \end{cases} \quad (70)$$

where the even part $r(t, x, v)$ and the odd part $j(t, x, v)$ of the flux $f(t, x, v)$ verify:

$$\begin{cases} r(t, x, v) = \frac{1}{2} (f(t, x, v) + f(t, x, -v)), \\ j(t, x, v) = \frac{1}{2\varepsilon} (f(t, x, v) - f(t, x, -v)). \end{cases} \quad (71)$$

It then follows that

$$f(t, x, v) = \begin{cases} r(t, x, v) + \varepsilon j(t, x, -v), & v \geq 0, \\ r(t, x, -v) - \varepsilon j(t, x, -v), & v < 0, \end{cases} \quad (72)$$

and

$$n = 2 \int_0^1 r dv.$$

Therefore, the vacuum boundary conditions are defined for $v > 0$ as:

$$\begin{cases} (r(t, x, v) + \varepsilon j(t, x, v))|_{x=-1} = 0, \\ (r(t, x, v) - \varepsilon j(t, x, v))|_{x=1} = 0. \end{cases} \quad (73)$$

When $\varepsilon \leq 1$, the parity system (70) can be rewritten as:

$$\begin{cases} \frac{\partial r}{\partial t} + v \partial_x j = \frac{1}{2\varepsilon^2} [(1 + \varepsilon |v \partial_x S|) n - (2 + \varepsilon |\partial_x S|) r], \\ \frac{\partial j}{\partial t} + v \partial_x r = \frac{1}{2\varepsilon^2} [(v \partial_x S) n - (2 + \varepsilon |\partial_x S|) j] + (1 - \frac{1}{\varepsilon^2}) v \partial_x r. \end{cases} \quad (74)$$

Taking the limit as $\varepsilon \rightarrow 0$ in (74), yields

$$j(t, x, v) = \frac{1}{2}(v\partial_x S)n - v\partial_x r.$$

Replacing j in (73) and taking into account the homogenous Neumann boundary condition prescribed on S , one obtains the following boundary condition:

$$\begin{cases} (r - \varepsilon v\partial_x r)|_{x=-1} = 0, \\ (r + \varepsilon v\partial_x r)|_{x=1} = 0. \end{cases} \quad (75)$$

The odd-even parity asymptotic preserving scheme for the initial kinetic equation consists of a two steps operator splitting method which combine an implicit scheme for the stiff collision term

$$\begin{cases} \frac{\partial r}{\partial t} = \frac{1}{2\varepsilon^2}[(1 + \varepsilon|v\partial_x S|)n - (2 + \varepsilon|\partial_x S|)r], \\ \frac{\partial j}{\partial t} = \frac{1}{2\varepsilon^2}[(v\partial_x S)n - (2 + \varepsilon|\partial_x S|)j] + (1 - \frac{1}{\varepsilon^2})v\partial_x r, \end{cases} \quad (76)$$

with an explicit scheme for the non stiff transport term

$$\begin{cases} \frac{\partial r}{\partial t} + v\partial_x j = 0, \\ \frac{\partial j}{\partial t} + v\partial_x r = 0. \end{cases} \quad (77)$$

For the spatial discretization, a center finite difference can be used for the collision step (76) and a second order upwind scheme for the transport step (77).

Numerical tests: In the following, we denote by:

- MM: the scheme obtained from the micro-macro decomposition,
- K-S: the scheme for the keller-Segel system,
- Explicit: the explicit scheme for the kinetic equation,
- Odd-Even: the odd-even parity asymptotic preserving scheme.

We have observed that the use of the time implicit discretization for the micro-macro model and the Keller-Segel limit give rise to numerical results which are very close to those produced by the explicit discretization. Hence, for the numerical results presented, we use the implicit approach for the MM and K-S schemes. The first test concerns the convergence order of the MM scheme computed at time t using the l^2 as :

$$e_{\Delta x}(f) = \frac{\|f_{\Delta x}(t) - f_{2\Delta x}(t)\|_2}{\|f_{2\Delta x}(0)\|_2}$$

where $f_{\Delta x}$ denotes the approximation of f using the spatial grid size Δx . The time step is set to $\Delta t = \frac{(\Delta x)^2}{2}$. Figure 1 presents the convergence rates obtained

with $N_x = 80, 160, 320, 640$ at time $t = 0.1$ for $\varepsilon \in \{1, 0.01, 10^{-4}, 10^{-6}\}$ and the total mass: $M = 2\pi$ (Figure 1). It can be seen that the MM scheme converges uniformly since time step does not depend on ε . A second order convergence is observed in the diffusive regime ($\varepsilon \leq 10^{-4}$).

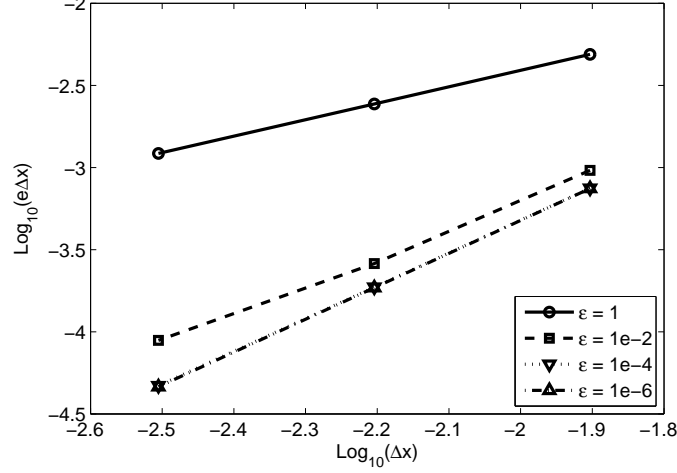


Figure 1: Convergence order of the method for $\varepsilon \in \{1, 0.01, 10^{-4}, 10^{-6}\}$ at time $t = 0.1$ ($M = 2\pi$).

In the following, we set $N_x = 200$, $M = 2\pi$. The time step is set to $\Delta t = \frac{\varepsilon \Delta x}{2}$ at the kinetic regime and $\Delta t = O(\Delta x)$ at the diffusive regime ($\Delta t = \Delta x/2$ for MM and K-S schemes and $\Delta t = \Delta x/40$ for the Odd-Even method). We mentioned that the comparison of the MM, Odd-Even and Explicit methods, the initial condition has been projected at the equilibrium for the last two methods at the kinetic regime. We illustrate in Figure 2 the behaviour of the MM scheme at different regimes. For different values of ε ($\varepsilon_k = 2^{-k}$, $k \geq 0$), we plot at time $t = 0.5$ the density of cells. We also add the result obtained with the K-S scheme. It can be seen that the MM scheme is stable as $\varepsilon \rightarrow 0$ and converges to the Keller-Segel limit. Indeed, for $\varepsilon \leq 2^{-7}$, the profiles of the density given by the two schemes are quite the same.

To check the behaviour of MM scheme in kinetic regime, we compare in Figure 3 the density of cells obtained for $\varepsilon = 1$ with the MM, Explicit and Odd-Even schemes at time $t = 0.5$. As expected, for both schemes, the results are very closed.

We also illustrate the behaviour of the methods in macroscopic regime. We compare in Figure 4 the density of cells obtained for $\varepsilon = 10^{-6}$ with the MM, Odd-Even K-S schemes at time $t = 0.5$. As expected, for both schemes, the results are quite the same.

We investigate the time evolution of the density using the MM scheme in different regimes ($\varepsilon = 1, 0.01, 10^{-6}$). The results are shown in Figures 5, 6 and

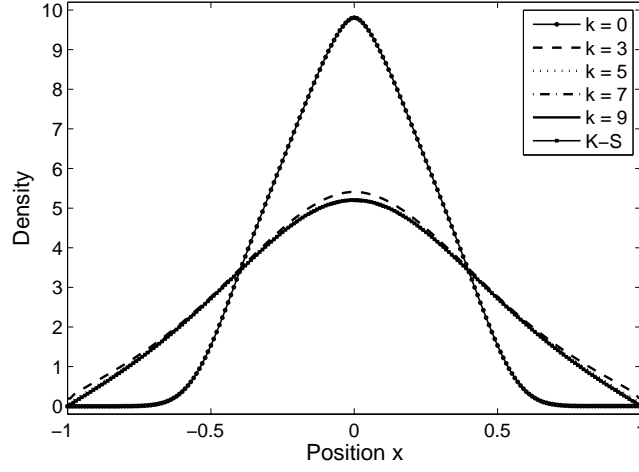


Figure 2: Density of cells at time $t = 0.5$ using MM and K-S schemes for $\varepsilon = 2^{-k}$ ($k \in \{0, 3, 5, 7, 9\}$) and $M = 2\pi$

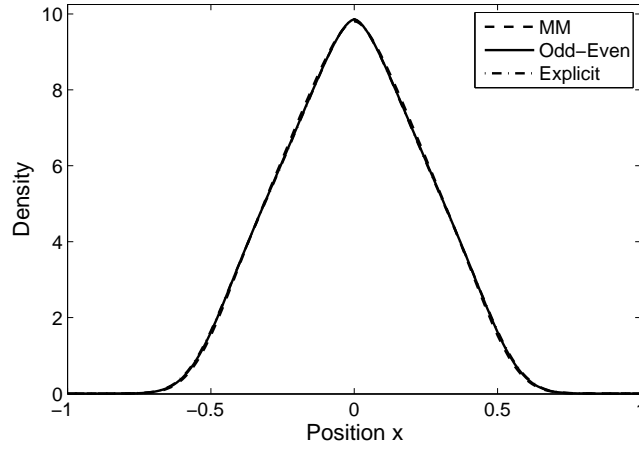


Figure 3: Density of cells at time $t = 0.5$ obtained with MM, Odd-Even and Explicit schemes for $\varepsilon = 1$ and $M = 2\pi$.

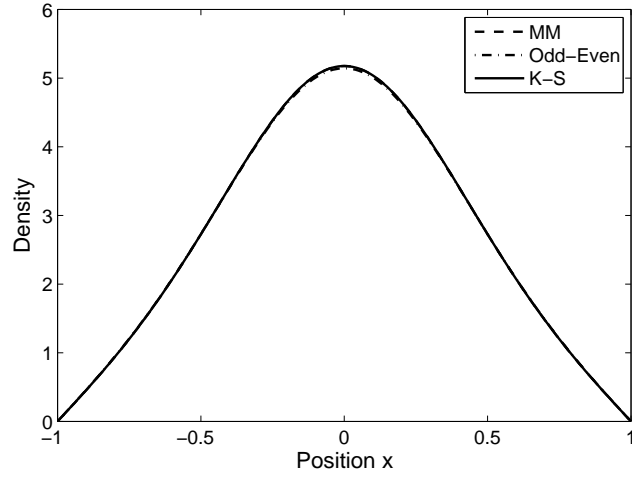


Figure 4: Density of cells at time $t = 0.5$ obtained with MM, Odd-Even and K-S schemes for $\varepsilon = 10^{-6}$ and $M = 2\pi$.

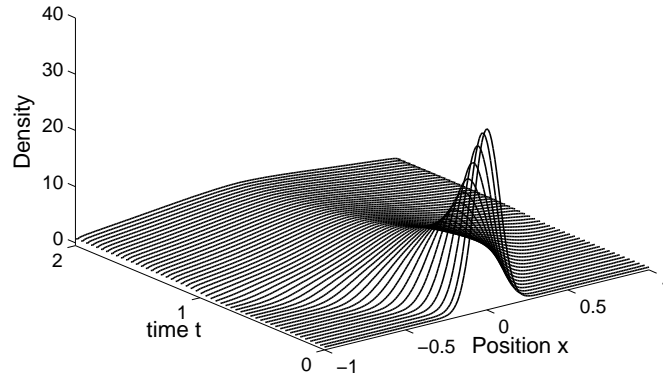


Figure 5: Evolution of the cell Density using MM scheme for $\varepsilon = 1$ and $M = 2\pi$.

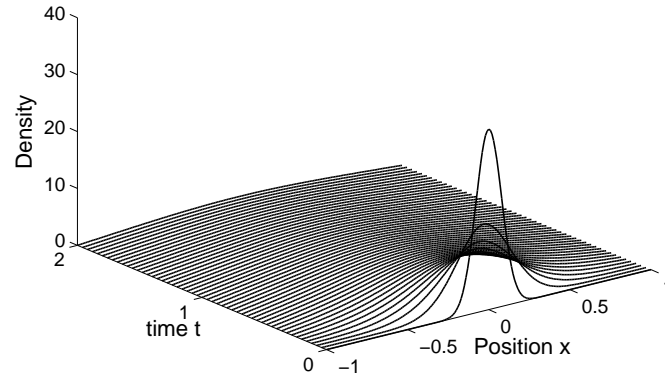


Figure 6: Evolution of the cell Density using MM scheme for $\varepsilon = 0.01$ and $M = 2\pi$.

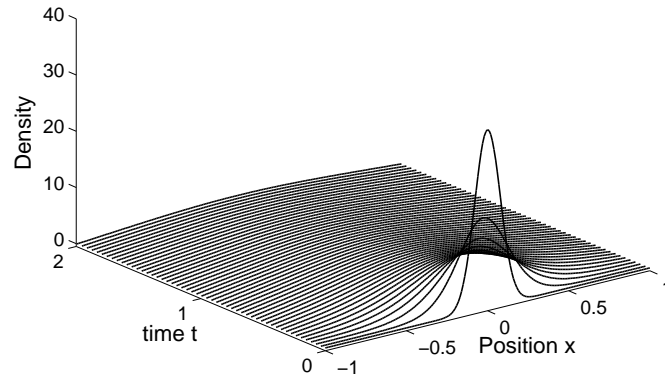


Figure 7: Evolution of the cell Density using MM scheme for $\varepsilon = 10^{-6}$ and $M = 2\pi$.

7. In each figure, the density seems to evolve to a stationary solution.

6 Closure looking ahead at research perspectives

This paper has developed a computational approach to a class of pattern formation models derived from the celebrated Keller-Segel model obtained by the underlying description delivered by generalized kinetic theory methods. The derivation is based on a decomposition with two scales, namely the microscopic and the macroscopic one technically related, as we have seen, by suitable small parameters accounting for the time and space dynamics.

The novelty of our paper is that the computational scheme follows precisely the derivation hallmarks by using the same decomposition and parameters. This idea improves the stability properties of the solutions with respect to classical approaches known in the literature. However, without repeating concepts already mentioned in the previous sections, we wish to stress that this method can contribute to future developments also related to applications. In fact, the need of new models in biology is well presented in [23] and [5] to account for a broad variety of biological phenomena. Moreover, it is shown in [5] that the so-called micro-macro decomposition can lead to an interesting variety of models such as models of angiogenesis phenomena.

Therefore, modeling and computational methods can march together thus contributing to a deeper understanding of the specific features of the two different, however, related fields. Indeed, we have in mind not only applications in biology, but also to the dynamics of self-propelled particles such as those of vehicular traffic as it has been recently shown [4] how macroscopic models can be derived from the kinetic description using precisely the micro-macro decomposition treated in this present paper.

Acknowledgments

The first author was supported by Hassan II Academy of Sciences and Technology (Morocco), project "Méthodes mathématiques et outils de modélisation et simulation pour le cancer". Part of this work was done during the visit of the second author at ENSA Marrakech (Morocco). He will like to thank the first author for the hospitality.

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